DATA INPUT INSTRUCTIONS FOR GROUND-WATER TRANSPORT PROCESS (GWT) Version (GWF1.7/GWT1.2)

[Derived from *MODFLOW-2000 (Version 1.1)* and *MOC3D (Version 3.5)*]

The solute-transport simulation package that is integrated with MODFLOW-2000 is called the Ground-Water Transport Process (GWT). It is derived directly from the *MOC3D* model (Konikow and others, 1996), which had been integrated with MODFLOW-96 (Harbaugh and McDonald, 1996). Following is a set of instructions for preparing an input data set for the **GWT** process. For more comprehensive descriptions of input parameters, options, and underlying assumptions, the user should also refer to Konikow and others (1996), Kipp and others (1998), Goode (1999), and Heberton and others (2000). One major change that has been implemented since the release of MOC3D Version 3.5 is the elimination of former item 18a, which was used to define the thickness of layers. This is no longer used because vertical discretization (and hence thickness) is now defined in the input data for MODFLOW-2000 (see Harbaugh and others, 2000). Another change is in the file type used in the MODFLOW name file. This version of the code is also compatible with the Lake and Gage Packages, the Constant-Head Boundary Package, and the Drain-Return Package.

MODFLOW Name File

Transport simulation is activated by including a record in the *MODFLOW* name file using the file type (Ftype) "GWT" to link to the transport name file. The transport name file specifies the files to be used when simulating solute transport in conjunction with a simulation of ground-water flow using *MODFLOW*. The transport name file works in the same way as the *MODFLOW* name file. (The Ftype "CONC" is not valid with MODFLOW-2000.)

MODFLOW Source and Sink Packages

Except for recharge and lakes, concentrations associated with fluid sources (C') are read as auxiliary parameters in the *MODFLOW* source package. The source concentration is read from a new column appended to the end of each line of the data file describing a fluid sink/source (see documentation for revised *MODFLOW* model; Harbaugh and McDonald, 1996a and 1996b). For example, concentrations associated with well nodes should be appended to the line in the WEL Package where the well's location and pumping rate are defined. These concentrations will be read if the auxiliary parameter "CONCENTRATION" (or "CONC") appears on the first line of the well input data file. The concentration in recharge is defined separately, as described in a following section, "Source Concentration in Recharge File." The preparation of input data files for using the Lake Package when solute-transport is also simulated is described in detail in the Lake Package documentation (Merritt and Konikow, 2000).

To simulate solute transport the *MODFLOW* option enabling storage of cell-by-cell flow rates for each fluid source or sink is required in all fluid packages except recharge. The key

word “CBCALLOCATE” (or “CBC”) must appear on the first line of each input data file for a fluid package (see Harbaugh and McDonald, 1996a and 1996b).

GWT Input Data Files

All input variables are read using free formats, except as specifically indicated. In free format, variables are separated by one or more spaces or by a comma and optionally one or more spaces. Blank spaces are not read as zeros. Variables that are optional are enclosed in brackets, as in {option}.

Ground-Water Transport Name File (GWT)

FOR EACH SIMULATION:

1. Data: FTYPE NUNIT FNAME

The name file consists of records defining the names and unit numbers of the files. Each “record” consists of a separate line of data. There must be a record for the listing file and for the main *GWT* input file.

The listing (or output) file (“CLST”) must be the first record. The other files may be in any order. Each record can be no more than 79 characters.

FTYPE The file type, which may be one of the following character strings:

CLST *GWT* listing file (separate from the *MODFLOW* listing file) *[required]*.

MOC or ***MOCIMP*** or ***ELLAM*** Main *GWT* input data file *[required]*. Specifying ***MOC*** indicates dispersion calculations will be explicit (as described by Konikow and others, 1996); specifying ***MOCIMP*** indicates dispersion calculations will be implicit (as described by Kipp and others, 1998); and specifying ***ELLAM*** indicates that the solute-transport equation will be solved using the *ELLAM* method (as described by Heberton and others, 2000).

CRCH Concentrations in recharge *[optional]*.

CNCA Separate output file containing concentration data in ASCII (text-only) format *[optional]*. Frequency and format of printing controlled by NPNTCL and ICONFM. If concentrations are written to a separate output file, they will not be written to the main output file.

CNCB Separate output file containing concentration data in binary format *[optional]*.

VELA Separate output file with velocity data in ASCII format *[optional]*. Frequency and format of printing controlled by NPNTVL and IVELFM.

VELB Separate output file with velocity data in binary format *[optional]*.

PRTA Separate output file with particle locations printed in ASCII format *[optional]*. Frequency and format of printing controlled by NPNTPL.

PRTB Separate output file with particle locations printed in binary format *[optional]*.

OBS Observation wells input file *[optional]*.

DATA For formatted files such as those required by the OBS package and for array data separate from the main *MOC3D* input data file *[optional]*.

DATA(BINARY) For formatted input/output files *[optional]*.

AGE Ground-water age simulation input file *[optional]*. (Not compatible with *ELLAM* option.)

DP Double porosity input file *[optional]*. (Not compatible with *ELLAM* option.)

DK Simple reactions(decay, zero-order growth, retardation) input file *[optional]*. (Not compatible with *ELLAM* option.)

CHFB Transport properties for Horizontal Flow Barriers and alternate calculation of dispersive flux near HFB cells *[optional]*. This option only should be used if the HFB package is active.

NUNIT The FORTRAN unit number used to read from and write to files. Any legal unit number other than 97, 98, and 99 (which are reserved by *MODFLOW*) can be used provided that it is not previously specified in the *MODFLOW* name file.

FNAME The name of the file.

Note: AGE, DP, and DK file types are described by Goode (1999). The CHFB file type is described by Hornberger and others (2002).

Files of type DATA and DATA(BINARY) can be designated as either input or output files. One of the options (either "OLD" for an input file or "REPLACE" for an output file) may be placed after the file name on the line listing the file type, unit number, and file name. If "OLD" is specified, the file must exist when the program is started. If "REPLACE" is specified and the file exists when the program is started, the existing file is deleted, then opened. The status of each file ("OLD", "REPLACE", or "UNKNOWN") is now shown in the output file. Note that the "OLD" or "REPLACE" option is not required. If neither is listed, the file status is shown as "UNKNOWN" and program execution continues normally. When output to a BINARY file from an earlier model run exceeds the amount of output generated by the current model run, specifying "REPLACE" may be required to ensure the file does not include output from the previous run after the output generated by the current run. The options may be entered in any combination of uppercase and lowercase letters.

Main *GWT* Package Input (*MOC, MOCIMP,* or *ELLAM*)

Input for the solute-transport package is read from the unit specified in the transport name file. The input consists of up to 19 separate items, as described in detail below (note that item numbers do not necessarily correspond with line numbers in the file). These data are used to specify information about the transport subgrid, physical and chemical transport parameters, numerical solution variables, and output formats. Output file controls for the *GWT* package are specified in the transport name file, described previously.

FOR EACH SIMULATION:

1. Data: HEDMOC — A two-line character-string title describing the simulation (80 text characters per line).

2. Data: HEDMOC (continued)

3. Data: ISLAY1 ISLAY2 ISROW1 ISROW2 ISCOL1 ISCOL2

ISLAY1 Number of first (uppermost) layer for transport.
ISLAY2 Last layer for transport.
ISROW1 First row for transport.
ISROW2 Last row for transport.
ISCOL1 First column for transport.
ISCOL2 Last column for transport.

Notes:

Transport may be simulated within a subgrid, which is a "window" within the primary *MODFLOW* grid used to simulate flow. Within the subgrid, the row and column spacing must be uniform if FTYPE *MOC* or *MOCIMP* are specified in the transport name file, but subgrid spacing can vary as in *MODFLOW* if *ELLAM* is specified. The thickness can vary from cell to cell and layer to layer. However, the range in thickness values (or product of thickness and porosity) should be as small as possible.

4. Data: NODISP DECAY DIFFUS

NODISP Flag for no dispersion (set NODISP = 1 if no dispersion in problem; this will reduce storage allocation).
DECAY First-order decay rate [1/T] (DECAY = 0.0 indicates no decay occurs).
DIFFUS Effective molecular diffusion coefficient [L^2/T].

Notes:

The decay rate (λ) is related to the half life ($t_{1/2}$) of a constituent by $\lambda = (\ln 2)/t_{1/2}$.

The effective molecular diffusion coefficient (D_m) includes the effect of tortuosity.

IF Ftype *MOC* OR *MOCIMP* IS ACTIVE:

5a. Data: NPMAX NPTPND

NPMAX Maximum number of particles available for particle tracking of advective transport in *MOC3D*. If set to zero, the model will calculate NPMAX according to the following equation:

$$NPMAX = 2 \times NPTPND \times NSROW \times NSCOL \times NSLAY.$$

NPTPND Initial number of particles per cell in transport simulation (that is, at $t = 0.0$). Valid options for default geometry of particle placement include 1, 2, 3, or 4 for one-dimensional transport simulation; 1, 4, 9, or 16 for two-dimensional transport simulation; and 1, 8, or 27 for three-dimensional transport simulation. The user can also customize initial placement of particles by specifying NPTPND as a negative number, in which case the minus sign is recognized as a flag to indicate custom placement is desired. In this case, the user must input local particle coordinates as described below.

IF Ftype *ELLAM* IS ACTIVE:

5b. Data: NSCEXP NSREXP NSLEXP NTEXP

NSCEXP Exponent used to calculate the number of subcells in the column direction (NSC, where NSC = 2**NSCEXP).

NSREXP Exponent used to calculate the number of subcells in the row direction (NSR).

NSLEXP Exponent used to calculate the number of subcells in the layer direction (NSL).

NTEXP Exponent used to calculate the number of sub-time steps per transport time increment (NT).

Notes:

In general, numerical accuracy will be increased by increasing the value of these parameters. This will also, however, increase computational costs. For each of the four parameters above, the value represents the exponent y in the expression 2^y.

Entering a zero or negative value for any of the above variables will cause the code to use default values. Default values for NSCEXP, NSREXP, and NSLEXP are 2 in active dimensions and 1 in inactive dimensions (for example, if a simulation represented a two-dimensional areal problem in which the number of rows and columns were greater than one and the number of layers equals one, then default settings would be NSCEXP = 2, NSREXP = 2, and NSLEXP = 1, and the number of subcells in each direction would be 4, 4, and 2, respectively). The default value of NTEXP is 2.

IF *MOC* OR *MOCIMP* IS ACTIVE AND IF *NPTPND* IS NEGATIVE IN SIGN:

6. Data: PNEWL PNEWR PNEWC

PNEWL Relative position in the layer (z) direction for initial placement of particle within any finite-difference cell.

PNEWR Relative position in the row (y) direction for initial placement of particle.

PNEWC Relative position in the column (x) direction for initial placement of particle.

Notes:

The three new (or initial) particle coordinates are entered sequentially for each of the NPTPND particles. Each line contains the three relative local coordinates for the new particles, in order of layer, row, and column. There must be NPTPND lines of data, one for each particle. The local coordinate system range is from -0.5 to 0.5, and represents the relative distance within the cell about the node location at the center of the cell, so that the node is located at 0.0 in each direction.

FOR EACH SIMULATION:

7. Data: CELDIS {FZERO} {INTRPL}

CELDIS Maximum fraction of cell dimension that particle may move in one step (typically, 0.5 ≤ CELDIS ≤ 1.0). For *ELLAM*, CELDIS can be greater than 1.0, and specifying CELDIS = 0.0 will result in one transport time step being used (which is not generally recommended).

FZERO If the fraction of active cells having no particles exceeds FZERO, the program will automatically regenerate an initial particle distribution before continuing the simulation (typically, 0.01 ≤ FZERO ≤ 0.05). Only specify if *MOC* or *MOCIMP* is active.

INTRPL Flag for interpolation scheme used to estimate velocity of particles. The default (INTRPL = 1) will use a linear interpolation routine; if INTRPL = 2, a scheme will be implemented that uses bilinear interpolation in the row and column (*j* and *i*) directions only (linear interpolation will still be applied in the *k*, or layer, direction). Only specify if *MOC* or *MOCIMP* is active. If *ELLAM* is specified, the code will automatically set INTRPL = 1.

IF *MOCIMP* IS ACTIVE:

7.1 Data: FDTMTH NCXIT IDIREC EPSSLV MAXIT

FDTMTH Weighting factor for temporal differencing of dispersion equation (0.0 ≤ FDTMTH ≤ 1.0). We suggest using either a value of FDTMTH = 0.5, a centered-in-time (or Crank-Nicolson) approximation, or FDTMTH = 1.0, a backward-in-time (or fully implicit) approximation. [Default value = 1]

NCXIT Number of iterations for the explicitly-lagged cross-dispersive flux terms (NCXIT ≥ 1). We suggest that the user initially specify a value of 2, but if the solution exhibits significant areas of negative concentrations, then the value of NCXIT should be increased to require more iterations, which typically will reduce the extent and magnitude of negative concentrations (at the cost of increased computational time). [Default value = 2]

IDIREC Direction index for permutation of the red-black node renumbering scheme. The order is as follows: 1: x,y,z; 2: x,z,y; 3: y,x,z; 4: y,z,x; 5: z,x,y; and 6: z,y,x. The first direction index is advanced most rapidly and the last direction index is advanced least rapidly. In some cases, there can be a significant variation in the number of iterations needed to achieve convergence, depending on the order of the directions for the red-black renumbering. We suggest that the user initially specify IDIREC = 1. If this leads to a relatively large number of iterations (more than 10), then the user should experiment with alternate choices to determine the one requiring the fewest number of iterations for their particular problem. [Default value = 1]

EPSSLV Tolerance on the relative residual for the conjugate-gradient solution of the matrix of the difference equations. We suggest that the user initially specify EPSSLV ≤ 10^{-5}. An adequately small value of EPSSLV has the property that a smaller value

does not change the numerical solution within the number of significant digits desired by the user. In the single-precision code implemented here, EPSSLV should not be less than 10^{-7}. [Default value = 10^{-5}]

MAXIT Maximum number of iterations allowed for the iterative solution to the difference equations for dispersive transport. In most cases, MAXIT = 100 is satisfactory. [Default value = 100]

Notes:

Entering a zero or out-of-range value for any of these five variables will cause the code to use the indicated default value.

FOR EACH SIMULATION:

8. Data: NPNTCL ICONFM NPNTVL IVELFM NPNTDL IDSPFM {NPNTPL}

NPNTCL Flag for frequency of printing concentration data. If NPNTCL = -2, concentration data will be printed at the end of every stress period; if NPNTCL = -1, data will be printed at the end of every flow time step; if NPNTCL = 0, data will be printed at the end of the simulation; if NPNTCL = N > 0, data will be printed every Nth particle moves, and at the end of the simulation. Initial concentrations are always printed. Solute budget and mass balance information are only printed every time concentration data are saved.

ICONFM Flag for output format control for printing concentration data. If concentration data are written to main output file (file type CNCA is not used), ICONFM represents a code indicating the format style (table 9, also see Harbaugh and McDonald, 1996a, p. 19). If concentration data are written to a separate output file (file type CNCA exists), specifying ICONFM $\geq$ 0 will indicate that concentration data are to be written as a matrix of values for each layer of the subgrid, whereas specifying ICONFM < 0 will indicate that concentration data are to be written as a table of values having one row for each node in the subgrid and four columns (x, y, z, and concentration), where x, y, and z are the actual nodal coordinates in the length units of the model simulation. Note that we follow the *MODFLOW* convention in that y increases from top to bottom row, and z increases from top layer to bottom layer. Also note that the x and y values are given with respect to the entire *MODFLOW* grid, but the z location is calculated only for vertical distances within the layers of the transport subgrid. If data are written in matrix style, one header line precedes and identifies the data for each layer. If data are written as a table of values, one header line is written each time that concentration data are saved.

NPNTVL Flag for printing velocity data. If NPNTVL = -1, velocity data will be printed at the end of every stress period; if NPNTVL = 0, data will be printed at the end of the simulation; if NPNTVL = N > 0, data will be printed every Nth flow time steps, and at the end of the simulation.

IVELFM Specification for format of velocity data, if being printed in main output file (see table 9).

NPNTDL Flag for printing dispersion equation coefficients that include cell dimension factors (see section "Program Segments"). If NPNTDL = -2, coefficients will be printed at the end of every stress period; if NPNTDL = -1, coefficients will be printed at the end of the simulation; if NPNTDL = 0, coefficients will not be printed; if NPNTDL = N > 0, coefficients will be printed every Nth flow time step.

IDSPFM Specification for format of dispersion equation coefficients (see table 1).

NPNTPL Flag for printing particle locations in a separate output file (only used if file types "PRTA" or "PRTB" appear in the *MOC3D* name file). If neither "PRTA" or "PRTB" is entered in the name file, NPNTPL will be read but ignored (so you must always have some value specified here). If either "PRTA" or "PRTB" is entered in the name file, initial particle locations will be printed to the separate file first, followed by particle data at intervals determined by the value of NPNTPL. If NPNTPL = -2, particle data will be printed at the end of every stress period; if NPNTPL = -1, data will be printed at the end of every flow time step; if NPNTPL = 0, data will be printed at the end of the simulation; if NPNTPL = N > 0, data will be printed every Nth particle moves, and at the end of the simulation. Only specify if *MOC* or *MOCIMP* is active.

Table 1. Formats associated with print flags. (Positive values for wrap format; negative values for strip format. Also see Harbaugh and McDonald, 1996, p. 19.)

Print flag	Format	Print flag	Format	Print flag	Format
0	10G11.4	7	20F5.0	14	10F6.1
1	11G10.3	8	20F5.1	15	10F6.2
2	9G13.6	9	20F5.2	16	10F6.3
3	15F7.1	10	20F5.3	17	10F6.4
4	15F7.2	11	20F5.4	18	10F6.5
5	15F7.3	12	10G11.4		
6	15F7.4	13	10F6.0		

FOR EACH SIMULATION:

9. Data: CNOFLO Concentration associated with inactive cells of subgrid (used for output purposes only).

FOR EACH LAYER OF THE TRANSPORT SUBGRID:

10. Data: CINT(NSCOL,NSROW) Initial concentration.
Module: U2DREL*

* Module is a standard *MODFLOW* input/output module.

FOR EACH SIMULATION, ONLY IF TRANSPORT SUBGRID DIMENSIONS ARE SMALLER THAN FLOW GRID DIMENSIONS:

11. Data: CINFL(ICINFL) C' to be associated with fluid inflow across the boundary of the subgrid.

Module: U1DREL*

Notes:

The model assumes that the concentration outside of the subgrid is the same within each layer, so only one value of CINFL is specified for each layer within and adjacent to the subgrid. That is, the size of the array (ICINFL) is determined by the position of the subgrid with respect to the entire (primary) *MODFLOW* grid. If the transport subgrid has the same dimensions as the flow grid, this parameter should not be included in the input data set. If the subgrid and flow grid have the same number of layers, but the subgrid has fewer rows or fewer columns, ICINFL = NSLAY. Values are also required if there is a flow layer above the subgrid and/or below the subgrid. The order of input is: C' for first (uppermost) transport layer (if required); C' for each successive (deeper) transport layer (if required); C' for layer above subgrid (if required); and C' for layer below subgrid (if required).

FOR EACH SIMULATION:

12. Data: NZONES Number of zone codes among fixed-head nodes in transport subgrid.

IF *NZONES* > 0:

Data: IZONE ZONCON

IZONE Value identifying a particular zone.

ZONCON Source concentration associated with nodes in the zone defined by IZONE above.

Notes:

Zones are defined within the IBOUND array in the BAS Package of *MODFLOW* by specifying unique negative values for fixed-head nodes to be associated with separate fluid source concentrations. Each zone is defined by a unique value of IZONE and a concentration associated with it (ZONCON). There must be NZONES lines of data, one for each zone. Note that values of IZONE in this list must be negative for consistency with the definitions of fixed-head nodes in the IBOUND array in the BAS Package. If a negative value of IBOUND is defined in the BAS package but is not assigned a concentration value here, *GWT* will assume that the source concentrations associated with those nodes equal 0.0.

If heads or source concentrations associated with fixed-head cells vary with time, the CHD or FHB packages should be used to simulate those cells and to specify the associated source concentrations using auxiliary variables. If the source concentration value for a given fixed-head cell is specified both here (in data set 12) and in CHD or FHB, the latter values will override the former values.

FOR EACH LAYER OF THE TRANSPORT SUBGRID IF *MOC* OR *MOCIMP* IS ACTIVE:

13. Data: IGENPT(NSCOL,NSROW) Flag to treat fluid sources and sinks as either "strong" or "weak."

Module: U2DINT*

* Module is a standard *MODFLOW* input/output module.

Notes:

Where fluid source is "strong," new particles are added to replace old particles as they are advected out of that cell. Where a fluid sink is "strong," particles are removed after they enter that cell and their effect accounted for. Where sources or sinks are weak, particles are neither added nor removed, and the source/sink effects are incorporated directly into appropriate changes in particle positions and concentrations. If `IGENPT` = 0, the node will be considered a weak source or sink; if `IGENPT` = 1, it will be a strong source or sink. See section on "Special Problems" and discussion by Konikow and Bredehoeft (1978).

IF *NODISP* ≠ 1 (If dispersion is included in simulation):

14. Data: `ALONG(NSLAY)` Longitudinal dispersivity.
Module: `U1DREL`*

15. Data: `ATRANH(NSLAY)` Horizontal transverse dispersivity.
Module: `U1DREL`*

16. Data: `ATRANV(NSLAY)` Vertical transverse dispersivity.
Module: `U1DREL`*

Notes:

Items 14-16 should include one value for each layer in subgrid.

FOR EACH SIMULATION:

17. Data: `RF(NSLAY)` Retardation factor (`RF` = 1 indicates no retardation).
Module: `U1DREL`*

Notes:

If `RF` = 0.0 in input, the code automatically resets it as `RF` = 1.0 to indicate no retardation.

FOR EACH LAYER OF TRANSPORT SUBGRID:

18. Data: `POR(NSCOL,NSROW)` Cell porosity.
Module: `U2DREL`*

Notes:

The porosity is input as a separate array for each layer of the transport subgrid. The product of thickness and porosity should not be allowed to vary greatly among cells in the transport subgrid.

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* Module is a standard *MODFLOW* input/output module.

Source Concentration in Recharge File (CRCH)

Concentrations in recharge, if the recharge package is used, are read from a separate unit specified in the *MOC3D* name file. This is defined using the file type (Ftype) "CRCH."

FOR EACH STRESS PERIOD, IF RECHARGE PACKAGE USED:

1. Data: INCRCH — Flag to reuse or read new recharge concentrations.

Notes:

Read new recharge concentrations if INCRCH ≥ 0. Reuse recharge concentrations from the last stress period if INCRCH < 0.

2. Data: CRECH(NSCOL,NSROW) — Source concentration associated with fluid entering the aquifer in recharge.

Module: U2DREL*

* Module is a standard *MODFLOW* input/output module.

Observation Well File (OBS)

Nodes of the transport subgrid can be designated as "observation wells." At each such node, the time, head, and concentration after each move increment will be written to a separate output file to facilitate graphical postprocessing of the calculated data. The input file for specifying observation wells is read if the file type (Ftype) "OBS" is included in the *GWT* name file.

FOR EACH SIMULATION, IF *OBS* PACKAGE USED:

1. Data: NUMOBS IOBSFL

NUMOBS Number of observation wells.

IOBSFL If IOBSFL = 0, well data are saved in NUMOBS separate files. If IOBSFL > 0, all observation well data will be written to one file, and the file name and unit number used for this file will be that of the first observation well in the list.

FOR EACH OBSERVATION WELL:

2. Data: LAYER ROW COLUMN UNIT

LAYER Layer of observation well node.

ROW Row of observation well node.

COLUMN Column of observation well node.

UNIT Unit number for output file.

Notes:

If NUMOBS > 1 and IOBSFL = 0, you must specify a unique unit number for each observation well and match those unit numbers to DATA file types and file names in the *GWT* name file. If IOBSFL > 0, you must specify a unique unit number for the first observation well and match that unit number to a DATA file type and file name in the *GWT* name file.

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